Non-equilibrium thermodynamics for functionals of current and density

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We study a stochastic many-body system maintained in an non-equilibrium steady state. Probability distribution functional of the time-integrated current and density is shown to attain a large-deviation form in the long-time asymptotics. The corresponding Current-Density Cramér Functional (CDCF) is explicitly derived for irreversible Langevin dynamics and discrete-space Markov chains. We also show that the Cramér functionals of other linear functionals of density and current, like work generated by a force, are related to CDCF in a way reminiscent of variational relations between different thermodynamic potentials. The general formalism is illustrated with a model example.

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1. Introduction Deriving probability distributions of relevant physical quantities for stochastic systems out of equilibrium is a complex problem of great interest for many experimental situations. The issue is difficult because of the complexity of non-equilibrium evolutions. In recent years, several models were proposed where such quantities could be computed. For example, the case of steady-state, non-equilibrium systems was studied in [1], using theoretical tools developed earlier [2, 3].

In the case when the stochastic system can be described by equations of hydrodynamic type, a special matrix-based formulation can be used [4], leading to a rich class of behaviors, including integrability [5], non-ergodicity and non-equilibrium phase transitions [6], and interesting connections to random matrix theory [7].

In the present work, we investigate generic stochastic systems out of equilibrium, in the large deviation limit, under the assumption of continuous symmetries for the space of trajectories. This allows the large deviation functional for density and currents to be derived, using a different approach than in [1, 6].

2. Langevin processes in symmetric spaces Consider a Langevin process given in a configuration space M by a stochastic equation

$$\dot{\eta}_i = F_i(\boldsymbol{\eta}) + \xi_i(t), \quad \langle \xi_i(t)\xi_j(t')\rangle = \delta_{ij}\delta(t-t'), \quad (1)$$

or equivalently by a path integral with a measure

$$dQ = Z^{-1} \exp\left\{-S[\boldsymbol{\eta}(\tau)]\right\} \mathcal{D}\boldsymbol{\eta}(\tau), \tag{2}$$

for stochastic paths (maps $\mathbb{R}_+ \to M)$ $\boldsymbol{\eta}(t)$, with $\mathcal{D}\boldsymbol{\eta}$, Z, and

$$S(\boldsymbol{\eta}) = (1/2) \int_0^t d\tau \left[\dot{\eta}_i - F_i(\boldsymbol{\eta}) \right] \left[\dot{\eta}_i - F_i(\boldsymbol{\eta}) \right]$$
 (3)

being the functional measure, a normalization factor, and the action, respectively. Hereafter, summation over repeated indices is assumed. We use rescaled units so that the temperature of the thermal bath, modeled by the Langevin term in (1), is equal to one. We are interested in large deviation $(t \to \infty)$ relations for stochastic trajectories of the process (1), in the case when the system exhibits continuous symmetries preserving the metric induced by the force field \boldsymbol{F} (isometries). For a compact representation of stochastic trajectories, we introduce the fluctuating density and current at a point \boldsymbol{x} of the trajectory's configuration space

$$\varrho(\boldsymbol{\eta}, \boldsymbol{x}) \equiv \frac{1}{t} \int_0^t d\tau \delta(\boldsymbol{x} - \boldsymbol{\eta}(\tau)), \tag{4}$$

$$J_i(\boldsymbol{\eta}, \boldsymbol{x}) \equiv \frac{1}{t} \int_0^t d\tau \dot{\eta}_i \delta(\boldsymbol{x} - \boldsymbol{\eta}(\tau)). \tag{5}$$

In the next section we will derive the large-deviation limit of the joint probability distribution function for ρ , \exists :

$$\mathcal{P}[\boldsymbol{J}(\boldsymbol{x}), \rho(\boldsymbol{x})] \equiv \langle \delta(\varrho - \rho)\delta(\boldsymbol{J} - \boldsymbol{J})\rangle_{\xi}. \tag{6}$$

We will show that in the $t \to \infty$ limit, it takes the form $\mathcal{P}(\boldsymbol{J}, \rho) \sim \exp[-t\mathcal{S}(\boldsymbol{J}, \rho)]$, where the CDCF is

$$S(\boldsymbol{J}, \rho) = \int_{M} d\boldsymbol{x} \frac{[\boldsymbol{F}\rho - \boldsymbol{J} - (1/2)\boldsymbol{\partial}\rho]^{2}}{2\rho}.$$
 (7)

We will also obtain a similar large-deviation result for discrete Markov processes.

The explicit large deviation result (7) can be immediately used to get thermodynamics-like relations for Crámer functions of derived objects. One introduces the vector and scalar potentials (which can also be interpreted as gauge fields, i.e. generators of continuous symmetry transformations mentioned above), V(x), A(x) and the corresponding charges

$$w_{\mathbf{A}}(\mathbf{J}) \equiv \int_{M} d\mathbf{x} A_{j}(\mathbf{x}) \mathbf{J}^{j}(\boldsymbol{\eta}; \mathbf{x}) = \frac{1}{t} \int_{0}^{t} d\tau \dot{\eta}^{j} A_{j}(\boldsymbol{\eta}),$$

$$u_{V}(\varrho) \equiv \int_{M} d\mathbf{x} V(\mathbf{x}) \varrho(\boldsymbol{\eta}; \mathbf{x}) = \frac{1}{t} \int_{0}^{t} d\tau V(\boldsymbol{\eta}(\tau)). \quad (8)$$

At $t \to \infty$, the joint p.d.f. $\mathcal{P}(w, u) \equiv \langle \delta(w - w_{\mathbf{A}}(\mathbf{I})) \delta(u - u_{V}(\varrho)) \rangle_{\xi}$ of $w_{\mathbf{A}}(\mathbf{I})$ and $u_{V}(\varrho)$ has the large deviation form $\mathcal{P}_{[\mathbf{A},V]}(w,u) \sim \exp(-t\mathcal{S}_{[\mathbf{A},V]}(w,u))$, where

$$S_{[\boldsymbol{A},V]}(w,u) = \inf_{w_{\boldsymbol{A}}(\boldsymbol{J})=w, u_{V}(\rho)=u} S(\boldsymbol{J},\rho).$$
 (9)

3. Derivation for the Langevin processes Using a standard representation for the Dirac δ -functional (6) gives for the probability $\mathcal{P}(\boldsymbol{J}, \rho) \sim$

$$\int \mathcal{D} \boldsymbol{A}(\boldsymbol{x}) \mathcal{D} V(\boldsymbol{x}) e^{-it \int d\boldsymbol{x} (\boldsymbol{A} \boldsymbol{J} + V \rho)} \int \mathcal{D} \boldsymbol{\eta}(t) e^{-S(\boldsymbol{\eta}; \boldsymbol{A}, V)},$$

$$S(\boldsymbol{\eta}; \boldsymbol{A}, V) = S(\boldsymbol{\eta}) - i \int_0^t d\tau \left(\dot{\boldsymbol{\eta}}^j A_j(\boldsymbol{\eta}) + V(\boldsymbol{\eta}) \right), \quad (10)$$

where $\mathcal{D}A(x)$, $\mathcal{D}V(x)$ are the standard field-theoretical notations for functional differentials/measures.

In the large deviation limit $(t \to \infty)$, the path integral in (10) is estimated as

$$\int \mathcal{D}\boldsymbol{\eta}(\tau)e^{-S(\boldsymbol{\eta};\boldsymbol{A},V)} \propto \exp\left(t\mathcal{F}(\boldsymbol{A},V)\right), \text{ where } (11)$$

$$\mathcal{F}(\boldsymbol{A}, V) = \int d\boldsymbol{x} \hat{\mathcal{L}}_{\boldsymbol{A}, V} \bar{\rho}(\boldsymbol{x}), \text{ and}$$
 (12)

$$\hat{\mathcal{L}}_{A,V} \equiv (1/2)\nabla_j \nabla_j - \nabla_j F_j + iV, \ \nabla_j \equiv \partial_j - iA_j, \quad (13)$$

with $\bar{\rho}(\boldsymbol{x})$ the normalized right-eigenvector of the ground state (lowest eigenvalue) for the Fokker-Planck operator $\hat{\mathcal{L}}_{\boldsymbol{A},V}$,

$$\hat{\mathcal{L}}_{A,V}\bar{\rho} = \lambda\bar{\rho}, \text{ and } \int d\boldsymbol{x}\bar{\rho}(\boldsymbol{x}) = 1.$$
 (14)

Applying further the saddle-point approximation for the functional integral in (10) with respect to \mathbf{A}, V , and using (10,11,12,13), we arrive at the following equations:

$$\boldsymbol{J}(x) = (\boldsymbol{F} + i\boldsymbol{A} - (1/2)\boldsymbol{\partial})\bar{\rho}(\boldsymbol{x}), \quad \bar{\rho} = \rho. \tag{15}$$

Solving (14,15) for \mathbf{A} , V and $\bar{\rho}$ and substituting the result back in the saddle expression for (10) yields (7). Note that the final result does not depend on λ , although it explicitly enters (14).

Notice that for the physical current, $\partial_i J_i = 0$, and the functional integration measure in (10) is invariant with respect to the gauge transformation, $A_j \to A_j + \partial_j \varphi$. In deriving (11,12) from (10), the gauge freedom was fixed by the requirement that the left eigenfunction of $\hat{\mathcal{L}}_{A,V}$ conjugated to the right eigenfunction, $\bar{\rho}$, equals unity.

- 4. Comments (i) The variational principle (9) establishes the optimal-fluctuation picture of the distributions $\mathcal{P}(w, u; t)$ at long times on the level of currents/densities: The relevant probability $\mathcal{P}(w, u; t)$ is determined by the probability $\mathcal{P}(\boldsymbol{J}, \rho; t)$ of the optimal distributions $(\boldsymbol{J}(\boldsymbol{x}), \rho(\boldsymbol{x}))$ of current and density that correspond to the maximal probability, provided they reproduce the correct set of rates (w, u) as in (9).
- (ii) Comparison of the probability of a stochastic trajectory η and its time-reversed counterpart, combined with the fact that the entropy production along η depends on the correspondent current distribution $\mathfrak{I}(\{\eta\},x)$ only, leads to the fluctuation theorem relation [9] for the CDCF

$$S(-\boldsymbol{J}, \rho) - S(\boldsymbol{J}, \rho) = 2w_{\boldsymbol{F}}(\boldsymbol{J}). \tag{16}$$

- (iii) The special choice of the gauge (15) has a simple geometric interpretation: solving a heat-kernel type equation for operator (13) with delta-function initial condition usually leads to a gaussian solution with increasing variance. However, it is possible to apply infinitesimal gauge transformations such that the solution remain singular at all times. The gauge (15) achieves this result.
- (iv) The fact that in the large time limit $t \to \infty$ it is possible to approximate the effective action with a quadratic form in the gauge fields (which is equivalent to (7)), can be traced back to the formal expansion of the (gauged) heat kernel [8]

$$\langle x|e^{tD}|x\rangle = (4\pi t)^{-d/2} [1 + ta_1 + \ldots],$$
 (17)

where $D = \nabla^{\dagger}_{\mu} \nabla^{\mu} + X$ is a gauged heat kernel in d dimensions, and a_1 is the first Seeley coefficient, $a_1 = -X - \omega(A_{\mu})$, with ω a quadratic form. This result holds for compact spaces; for a generalization to spaces with (possibly fractal) boundary, see [10].

- (v) The result (7) can also be understood in very general terms starting with the problem of computing the current algebra (and hamiltonian) of sigma models in symmetric spaces (a field theory for maps into Riemann spaces with simple compact isometry group). In this setup, the force field \mathbf{F} provides a metric, and the continuous symmetry group preserves the metric. It is known [11] that the functional of currents for this theory has the form (7). This result was also used in the context of mesoscopic transport theory [12].
- 5. Derivation for irreversible Markov chains Irreversible Markov Chain (MC) stochastic dynamics can be viewed as a discrete (regularized) counterpart of the Langevin processes, that also occur in continuous time. We start with formulating the MC dynamics such that the formalism reported above can be applied with only minor changes. The configuration space M is a graph that consists of vertices $a \in M_0$ and edges $\{a, b\} \in M_1$. An edge $\{a,b\}$ will be further denoted $a \to b$ or $b \leftarrow a$. A Markov process is determined by a set of rates $k_{ab} \neq k_{ba}$ that reside on the graph edges. A discretized stochastic trajectory $\eta = (a_n, \dots, a_0; \tau_n, \dots, \tau_1)$ with $a_{j+1} \to a_j$ and $0 < \tau_1 < \ldots < \tau_n < t$ represents a set of instantaneous jumps from a_{j-1} to a_j that occur at times τ_j respectively. The Markovian measure $\mathcal{D}\eta \exp(-S(\eta))$, with $\mathcal{D}\boldsymbol{\eta} = \sum_n d\tau_1 \dots d\tau_n$, is described by the action

$$\exp(-S(\boldsymbol{\eta})) = \prod_{j=1}^{n} k_{a_j a_{j-1}} e^{-\sum_{i=0}^{n} \kappa_{a_i} (\tau_{i+1} - \tau_i)}, \quad (18)$$

where $\kappa_a = \sum_{b \to a} k_{ba}$ is the rate of leaving the site a.

Similar to (4,5), we can define the density $\rho_a(\eta)$ and the current $J_{ab}(\eta)$ associated with a trajectory η , as the relative portion of time spent on a, and the number of jumps $b \to a$ minus the number of jumps $a \to b$ divided by t, respectively. If a trajectory is closed we have the

current conservation $\sum_{b\to a} J_{ba}(\eta) = 0$. Correspondingly, functionals $u_V(\rho), w_{\boldsymbol{A}}(\boldsymbol{J})$ represent the time-average of function $V: M_0 \to \mathbb{R}$ relative to the distribution ρ , and the weighted average of function $\boldsymbol{A}: M_1 \to S_1$ (the unit circle), with respect to the distribution of jumps \boldsymbol{J} .

The variational principle (9) for the discrete case can be derived exactly in the same fashion as for the continuous case using the integration measures $\mathcal{D}V = \prod_a dV_a$, and $\mathcal{D}A = \prod_{a\to b} (2\pi i z_{ab})^{-1} dz_{ab}$. The fields V and A arise, as in (10), from the representation of Dirac's distribution for (6). The integrations dV_a and dz_{ab} go over the real axis and the unimodular circle $|z_{ab}| = 1$, respectively. As in the continuous case, the CDCF $\mathcal{S}(J, \rho)$ can be computed using the Fokker-Plank (FP) approach, which results in the expression (13) with the modified FP operator

$$\hat{\mathcal{L}}_{\mathbf{A},V} = \sum_{ab} k_{ab} z_{ab} \hat{\sigma}_{ab} - \sum_{a} (\kappa_a + V_a) \hat{\sigma}_{aa}, \qquad (19)$$

where $\hat{\sigma}_{ab} = |a\rangle\langle b|$. Note that for J, V = 0, the operator $\hat{\mathcal{L}}$ represents the rate matrix of the master equation, so $\hat{\mathcal{L}}_{A,V}$ can be referred to as the modified rate matrix.

Similar to the continuous case, the functional $S(J, \rho)$ can be identified explicitly, by fixing the gauge using conditions $\psi_{A,V} = \rho_a$ and $\mathcal{F}(A,V) = 0$. Thus, ρ is the zero mode of the modified FP operator (19). This results in:

$$S(\boldsymbol{J}, \rho) = \sum_{ab} J_{ab} \zeta_{ab} + \sum_{a} \rho_a V_a, \qquad (20)$$

$$J_{ab} = k_{ab} z_{ab} \rho_b - k_{ba} z_{ba} \rho_a = k_{ab} z_{ab} \rho_b - k_{ba} z_{ab}^{-1} \rho_a,$$
 (21)

with $\zeta_{ab} = \ln(z_{ab})$. We further make use of (21) to express z_{ab} in terms of (\boldsymbol{J}, ρ) and of the gauge fixing condition $\mathcal{F}(\boldsymbol{A}, V) = 0$ combined with the explicit form of the modified FP operator (19) to find an explicit expression for V_a . Upon substitution of these expressions into (20) we arrive at the explicit expression for the CDCF

$$S(J,\rho) = \sum_{a} \kappa_{a} \rho_{a} - \sum_{ab} \sqrt{J_{ab}^{2} + 4k_{ab}k_{ba}\rho_{a}\rho_{b}} + \sum_{ab} J_{ab} \ln \frac{\sqrt{J_{ab}^{2} + 4k_{ab}k_{ba}\rho_{a}\rho_{b}} + J_{ab}}{2k_{ab}\rho_{b}}.$$
 (22)

The variational principle can be applied to calculate the long-time distributions of the production rates for the observables represented as linear functions of current/density. In particular we have for the entropy production rate:

$$w(\mathbf{J}) = \sum_{ab} J_{ab} \ln \left(k_{ab} / k_{ba} \right). \tag{23}$$

6. Non-equilibrium thermodynamics for systems of identical particles In this section we illustrate how to derive a single-particle, coarse-grained, version of (7).

This is a potentially productive approach for addressing steady, non-equilibrium situations in stochastic systems of interacting particles [13, 14, 15].

Consider a system of N interacting Langevin processes,

$$\dot{\eta}_i = F_i(\eta_1, \cdots, \eta_N) + \xi_i(t), \quad \eta_i \in \mathbb{R}^1.$$
 (24)

We introduce the multi-point density and currents depending on all trajectories $\{\eta_i(\tau)\}_{i=1}^N$ and markers $\{x_i\}_{i=1}^N$

$$\varrho^{(N)} \equiv \frac{1}{t} \int_0^t d\tau \prod_{k=1,\dots,N} \delta \left(\eta_k(\tau) - x_k \right), \qquad (25)$$

$$\mathbf{J}_{i}^{(N)} \equiv \frac{1}{t} \int_{0}^{t} d\tau \dot{\eta}_{i}(\tau) \prod_{k=1,\dots,N} \delta\left(\eta_{k}(\tau) - x_{k}\right). \quad (26)$$

The multi-point effective action (7) for the joint p.d.f. of the multi-point density and currents, $\langle \delta(\rho^{(N)} - \varrho^{(N)}) \prod_{i=1}^{N} \delta(J_i^{(N)} - \beth_i^{(N)}) \rangle \propto \exp(-tS^{(N)})$, is

$$S^{(N)} = \sum_{k} \int \frac{d^{N} \mathbf{x}}{\rho^{(N)}} \left[F_{k} \rho^{(N)} - J_{k}^{(N)} - \frac{\partial_{x_{k}} \rho^{(N)}}{2} \right]^{2}. \quad (27)$$

Averages over $i, \varrho^{(0)} \equiv \frac{1}{Nt} \int_0^t d\tau \sum_k \delta\left(\eta_k(\tau) - x\right), \, \gimel^{(0)} \equiv \frac{1}{Nt} \int_0^t d\tau \sum_k \dot{\eta}_k(\tau) \delta\left(\eta_k(\tau) - x\right)$ describe single-particle density/currents. The effective action that controls the long-time asymptotic of the single-point p.d.f. $\langle \delta(\rho^{(0)} - \varrho^{(0)}) \delta(J^{(0)} - \gimel^{(0)}) \rangle \propto \exp(-tS^{(0)})$ is related to the multipoint action (27) via the exact variational relation

$$S^{(0)} = \inf_{\rho^{(N)}, J_1^{(N)}, \dots, J_N^{(N)}} S^{(N)} \Big|_{\Xi}$$
 (28)

$$\Xi = \left\{ \begin{array}{l} \rho^{(0)}(x) = N^{-1} \int \prod_i dx_i \sum_k \rho^{(N)} \delta(x_k - x) \\ J^{(0)}(x) = N^{-1} \int \prod_i dx_i \sum_k J_k^{(N)} \delta(x_k - x) \end{array} \right..$$

This can be derived by looking for the minimum of (27), subject to constraints (28), using Lagrange multipliers.

We now show how to derive asymptotic results for this example of a many-body system of interacting particles on a circle, with nearest-neighbor interactions, for a constant force field F. Starting from the discrete version of the model, we will consider the hydrodynamic limit $N \to \infty$ and obtain a smooth continuum model. Equations for interacting Langevin processes $\{\phi_i \in S_1\}_{i=1}^N$ are

$$\dot{\phi}_i = uN(\phi_i - \phi_{i-1}) + vN^2(\phi_{i+1} + \phi_{i-1} - 2\phi_i) + F + \xi_i(t),$$

with u,v effective parameters fixed by the interaction. In order to consider the hydrodynamic $N\to\infty$ limit, we introduce the field $\varphi(i,t)$ whose value at i is the Langevin process ϕ_i . A similar construction gives the noise field $\xi(i,t)$. In the hydrodynamic limit, the indices form a continuum, $\frac{i}{N}\to y\in S_1$ and the evolution is given by

$$\dot{\varphi}(y,t) = u \frac{\partial \varphi(y,t)}{\partial y} + v \frac{\partial^2 \varphi(y,t)}{\partial y^2} + F + \xi(y,t). \tag{29}$$

We can now apply the formalism presented earlier to compute the current $J^{(0)}$ in the continuum limit. It will

depend on the connectivity component, n. This integer parameter allows to separate particles in groups according to the number of expected full cycles completed in the large time limit. To illustrate this, consider runners on a circular track, and separate the group which completes between n and n+1 turns in a given time. We call that group a component, characterized by the integer n.

Performing a twisted Fourier decomposition

$$\varphi(y,t) = ny + \varphi_0(t) + \sum_{k=1}^{\infty} \left[a_k(t)e^{iky} + b_k(t)e^{-iky} \right], (30)$$

allows the minimization in (28) to be performed explicitly. This results in a set of Crámer functions for current J and density $\rho(\varphi)$, labeled by n

$$S_n^{(0)}(J,\rho) = N \oint \frac{d\varphi}{2\rho} \left[(F + un)\rho - J - \frac{1}{2}\partial_{\varphi}\rho \right]^2$$
 (31)

By symmetry, minimization with respect to ρ in (31) yields $\rho(\varphi) = 1$, and results in Gaussian distributions for J, peaked at F + un. The time-averaged current does not depend on the parameter v, which describes the diffusive part of the process, but only on u, which is related to drift around the circle. This is a natural conclusion upon analyzing averages of derivatives for (30): except for the linear term ny, all others average to zero due to their oscillatory nature. Hence, contributions are expected only from the terms depending on first-order derivatives.

- 7. Notes on further potential applications Turbulence is often modeled via a set of stochastically driven differential equations, which can be regularized in terms of interacting Lagrangian particles subjected to stochastic stirring and damping. Thus, a model describing the 3D evolution of a representative turbulent blob in terms of four-point configurations was presented in [16]. Considering coordinates and momenta of the Lagrangian particles as degrees of freedom, one maps the particle system onto the general model (1). Analyzing various functionals of relevant densities and currents (introduced for both the coordinates and momenta of the Lagrangian particles) and relating them to standard objects of interest in stochastic hydrodynamics, e.g., distribution functions of energy and density fluxes in momentum space, constitutes an intriguing new direction for future research.
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Note After the research described in this Letter was completed, we have learned about similar results obtained recently in [17]. Unlike in this work, they were obtained using a standard formulation [3]. We emphasize that our approach is different and allows more general types of interactions between Langevin processes.

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